

Microscopic analog of temperature within nonextensive thermostatistics

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Abstract

It is presented a microscopic interpretation for the temperature within Tsallis thermostatistics, generalizing the classical derivation based on the Boltzmann-Gibbs statistics. It is shown that with this definition the zeroth law and the equipartition theorem are valid in their classical form. Moreover, it is observed that the equation of state for an ideal gas within generalized thermostatistics preserves the classical Boyle's law form $PV = NkT$.

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I. INTRODUCTION

The explanation of the macroscopic theory of thermodynamics in terms of the more abstract microscopic statistical mechanics is one of the major achievements of the physics of the early twentieth century. This task included the establishment of connections between the macroscopic *state variables* and their microscopic counterparts. Among the thermodynamics variables, the *external parameters*, e.g. the volume of a gas, and the mechanical related quantities, e.g. the pressure, are easily interpreted microscopically. However, the non-mechanical thermodynamical quantities, viz., temperature, entropy and their various subsidiary quantities, are more cumbersome to identify microscopically, since they are basically defined within thermodynamics, with no apparent macroscopic mechanical equivalent quantity. The statistical mechanical analogues of temperature and entropy are characteristic quantities of the ensemble distribution.

The concept of temperature of a body lies in the very root upon which the whole science of thermodynamics rests. It is connected to our common sense of “hot” and “cold”, and the zero law of thermodynamics is the statement that this quantity can be compared by observing the behavior of bodies put in contact to each other. In statistical mechanics the temperature can be related, via the theorem of equipartition of energy, to the amount of kinetic energy per degrees of freedom of the system. Within the Boltzmann-Gibbs (BG) approach, it is also associated with the β constant that appears in the exponent of the canonical distribution.

An alternative formalism to the Boltzmann-Gibbs thermodynamics development has been evolved in the last decade starting from the postulate of a generalized entropy form by Tsallis [1]. Since then, a wealthy scientific bibliography has been produced presenting theoretical and experimental confirmation of the generalized thermostatistics. For a full and updated list of publications check [2].

It has been pointed out by Plastino [3] that systems with a small number of particles obey the generalized thermostatistics. Moreover, it has been proven by Almeida [4] that both formalisms (Boltzmann-Gibbs and Tsallis) can be obtained via a common logical development based on the hypothesis of equiprobability on phase space, ergodicity and the use of structure functions.

Our goal in this paper is to present a microscopic interpretation for the temperature within

Tsallis thermostatistics, generalizing the classical interpretation derived on the Boltzmann-Gibbs formulation. This endeavor has been already considered by Martinez et. al. [5, 6] and Plastino et. al. [7]. However, our presentation, which is based on elementary techniques of statistical mechanics, leads to the resolution of disparities with the classical Boltzmann-Gibbs approach that were encountered in these papers.

II. PRELIMINARY CONSIDERATIONS

Consider a system \mathcal{G} with Hamiltonian $H = H(\mathbf{q}, \mathbf{p})$ and let Ξ denote its phase space. Let $V(E)$ be the volume of the region of the phase-space where $H(\mathbf{q}, \mathbf{p}) < E$, and let $\Omega(E) = \partial V(E)/\partial E$ denote the *structure function* [8], also known as density of states. Let's define the function

$$\beta(E) = \frac{d}{dE} \ln \Omega(E). \quad (1)$$

Let the system \mathcal{G} be composed by two subsystems \mathcal{G}_1 and \mathcal{G}_2 with phase spaces Ξ_1 and Ξ_2 , respectively. For $i = 1, 2$, let's denote by $V_i(E)$ the volume function in the phase space Ξ_i of the region where $H_i(\mathbf{q}_i, \mathbf{p}_i) < E$, $\Omega_i(E)$ its respective structure function and $\beta_i(E)$ the associated beta function.

If \mathcal{G}_1 and \mathcal{G}_2 are in *weak interaction* with each other, in the sense that $H(\mathbf{q}, \mathbf{p}) = H_1(\mathbf{q}_1, \mathbf{p}_1) + H_2(\mathbf{q}_2, \mathbf{p}_2)$, i.e., there is no term of interaction of \mathcal{G}_1 with \mathcal{G}_2 in the Hamiltonian, then the canonical distribution of the system \mathcal{G}_1 in its phase space Ξ_1 , when the total energy of \mathcal{G} is $E = a$, is given by the density function [8]

$$\rho_1(E_1) = \frac{\Omega_2(a - E_1)}{\Omega(a)}, \quad (2)$$

and the structure function of the system \mathcal{G} satisfies the convolution relation

$$\Omega(E) = \int_0^E \Omega_1(\xi) \Omega_2(E - \xi) d\xi. \quad (3)$$

It has been shown in [4] that the form of ρ_1 depends on the value of the parameter q_2 determined by

$$\frac{d}{dE} \left(\frac{1}{\beta_2(E)} \right) = q_2 - 1. \quad (4)$$

When $q_2 = 1$, ρ_1 is an exponential (Boltzmann-Gibbs) and, when $q_2 \neq 1$, ρ_1 is a power-law (Tsallis) distribution. The function $V_2(E)$ can be obtained integrating Eq. (4). Let's

assume that all of the volume functions $V_i(E)$ are such that $V_i(0) = \Omega_i(0) = 0$. Therefore, the general form of $V_2(E)$ is

$$V_2(E) = C_2 E^{q_2/(q_2-1)}, \quad (5)$$

with C_2 a constant. An analogous procedure for the subsystem \mathcal{G}_1 yields

$$V_1(E) = C_1 E^{q_1/(q_1-1)}, \quad (6)$$

with C_1 a constant. Hence, for $i = 1, 2$,

$$\Omega_i(E) = \frac{q_i C_i}{q_i - 1} E^{1/(q_i-1)}, \quad (7)$$

and

$$\beta_i(E) = \frac{1}{(q_i - 1)E}. \quad (8)$$

From Eq. (3) we get that

$$\Omega(E) = C_1 C_2 \frac{\Gamma\left(\frac{q_1}{q_1-1} + 1\right) \Gamma\left(\frac{q_2}{q_2-1} + 1\right)}{\Gamma\left(\frac{q}{q-1}\right)} E^{1/(q-1)}, \quad (9)$$

where

$$\frac{q}{q-1} = \frac{q_1}{q_1-1} + \frac{q_2}{q_2-1}, \quad (10)$$

and $\Gamma(x)$ is the gamma function. The function β for \mathcal{G} is then given by

$$\beta(E) = \frac{1}{(q-1)E}. \quad (11)$$

From Eq. (9) we get that

$$V(E) = C_1 C_2 \frac{\Gamma\left(\frac{q_1}{q_1-1} + 1\right) \Gamma\left(\frac{q_2}{q_2-1} + 1\right)}{\Gamma\left(\frac{q}{q-1} + 1\right)} E^{q/(q-1)}. \quad (12)$$

The interpretation of the temperature is exactly the one based upon the theorem of equipartition of energy for the system \mathcal{G} with total energy $E = a$, which might be expressed [9] in the form

$$\left\langle x_i \frac{\partial H}{\partial x_j} \right\rangle = \delta_{ij} \frac{V(a)}{\Omega(a)} = \delta_{ij} kT \quad (13)$$

where x_i stands for any of the variables p_i or q_i , k is the Boltzmann constant and T is the absolute temperature. This is the same temperature definition for the Boltzmann-Gibbs

setting. Using the expressions for $V(a)$ and $\Omega(a)$, Eqs. (12) and (9) respectively, and the definition of β , Eq. (1), we may write the temperature of the system \mathcal{G} as

$$T = \frac{1}{k} \left(\frac{q-1}{q} \right) a = \frac{1}{kq\beta(a)}. \quad (14)$$

For a general system, we postulate that the function

$$\mathcal{T}(\mathcal{G}) = \frac{1}{kq} \left\langle \frac{1}{\beta(E)} \right\rangle \quad (15)$$

represents the physical temperature of the system \mathcal{G} . Note that \mathcal{T} is a function that depends on the observed part of the system. For the whole system \mathcal{G} with constant energy $E = a$, we have that $\beta(a) = ((q-1)a)^{-1}$ and

$$\mathcal{T}(\mathcal{G}) = \frac{1}{k} \left(\frac{q-1}{q} \right) a = T. \quad (16)$$

Consider now the subsystem \mathcal{G}_1 , which has a random energy E_1 distributed according to a probability density function [8][§15, pp. 75]

$$\frac{\Omega_1(x)\Omega_2(a-x)}{\Omega(a)}. \quad (17)$$

Therefore, the average value of the energy E_1 is

$$\langle E_1 \rangle = \frac{1}{\Omega(a)} \int_0^a x \Omega_1(x) \Omega_2(a-x) dx \quad (18)$$

$$= \frac{B\left(\frac{q_1}{q_1-1} + 1, \frac{q_2}{q_2-2}\right)}{B\left(\frac{q_1}{q_1-1}, \frac{q_2}{q_2-2}\right)} a \quad (19)$$

$$= \left(\frac{q_1}{q_1-1} \right) \left(\frac{q-1}{q} \right) a, \quad (20)$$

where $B(m, n)$ is the beta function. Then, from Eq. (15) we get the value

$$\mathcal{T}(\mathcal{G}_1) = \frac{1}{kq_1} \left\langle \frac{1}{\beta(E_1)} \right\rangle \quad (21)$$

$$= \frac{1}{k} \left(\frac{q_1-1}{q_1} \right) \langle E_1 \rangle = \frac{1}{k} \left(\frac{q-1}{q} \right) a \quad (22)$$

$$= \mathcal{T}(\mathcal{G}), \quad (23)$$

which shows that the evaluation of \mathcal{T} over any of the subsystems \mathcal{G}_i produces the same result.

Let's consider now the combination (*weakly interaction*) of two systems \mathcal{G}_1 and \mathcal{G}_2 , with parameters q_1 and q_2 respectively, to form a compound system \mathcal{G} . Let's impose the condition that before the assembling $\mathcal{T}(\mathcal{G}_1) = \mathcal{T}(\mathcal{G}_2)$, i.e.,

$$\left(\frac{q_1 - 1}{q_1} \right) a_1 = \left(\frac{q_2 - 1}{q_2} \right) a_2, \quad (24)$$

where a_1 and a_2 are the initial energies of the systems \mathcal{G}_1 and \mathcal{G}_2 respectively. Thus, the compound system \mathcal{G} has energy $a = a_1 + a_2$ and parameter q related to q_1 and q_2 by Eq. (10). Therefore, computing $\mathcal{T}(\mathcal{G})$ using Eq. (15) we have

$$\mathcal{T}(\mathcal{G}) = \frac{1}{k} \frac{a}{\left(\frac{q}{q-1} \right)} = \frac{1}{k} \left(\frac{a_1 + a_2}{\frac{q_1}{q_1-1} + \frac{q_2}{q_2-1}} \right) = \frac{1}{k} \frac{a_1}{\left(\frac{q_1}{q_1-1} \right)} = \mathcal{T}(\mathcal{G}_1) \quad (25)$$

$$= \frac{1}{k} \frac{a_2}{\left(\frac{q_2}{q_2-1} \right)} = \mathcal{T}(\mathcal{G}_2), \quad (26)$$

which implies that $\mathcal{T}(\mathcal{G})$, considered as a temperature scale, satisfies the *zero law of thermodynamics*.

III. APPLICATION

Consider now a system composed by N free particles in a confined three-dimensional volume V , i.e., an ideal gas system. It has been stated by Plastino and Lima [7] that the virial theorem in the generalized thermostatistics context leads to an equation of state for the ideal gas that is different from the usual Boyle's law; The Boyle's law being recovered in the limit case of $q \rightarrow 1$. This conflicting result was generated by the adoption of the temperature T as inverse of β divided by the Boltzmann constant, $T = (k\beta)^{-1}$. If instead of this we define the temperature by the relation Eq. (15) we assure a priori the validity of the equipartition theorem in its classical form Eq. 13). The classical virial theorem for the ideal gas [10] states that

$$\sum_i q_i F_i = -P \oint_S \mathbf{r} \cdot d\mathbf{S} = -3PV, \quad (27)$$

where \mathbf{r} is the position vector of a particle and F_i is the generalized i force associated to q_i . Therefore, the definition of temperature by Eq. (15) together with the classical virial theorem leads to the Boyle's law in its original form,

$$PV = NkT, \quad (28)$$

even in the context of the generalized thermostatistics.

IV. CONCLUSION

We have presented a microscopic identification of the temperature valid for both Boltzmann-Gibbs and Tsallis statistics. It was observed that the zeroth law of thermodynamics, the theorem of equipartition, and the equation of state for ideal gas are all valid in their classical form even within Tsallis framework, provided the adequate definition of temperature is taken. The adoption of an inadequate form of the temperature leads to conflicting results obtained by the BG and the Tsallis thermostatistics, e.g. the modified Boyle's law deduced in [7].

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